Optimization of a Chemical Production Facility: A study of operating conditions, equipment sizing, and economics of an ethylbenzene production plant.

by

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Abstract

Economics of a chemical plant depend on multiple factors: grade of a feed, types of catalyst, operating temperature and pressure, cost of equipment, and many other factors could have influences on economics of the plant. In a previous study about an ethylbenzene facility, our team scrutinize two proposed changes. An optimization plan is recommended by our team in order to maximize the net present value (NPV) of the plant. This report focuses on demonstrating rationales of setting certain operating conditions, showcasing the details of optimization, and elucidating the reasons behind applying these modifications. The team used simulating software PRO/-II to investigate various changes applied, and used CAPCOST for economic estimation. Even though any plant in the real world cannot be perfect, our result is a good starting point for more comprehensive and precise design. After the investigation, we conclude that reaction section, cooling section, recycle, and separating section can be optimized in order to keep the plant working in a highly efficient and effective manner. By manipulating operating conditions and equipment sizing, the entire plant is simplified and the ethylbenzene production process becomes more efficient than the original process. Furthermore, the net present value of the plant is increased dramatically, post-optimization.

Contents

List of Tables

List of Figures

Chapter 1
Introduction

Engineers are trained and hired to solve real-world problems, and in many cases, engineers evaluate and optimize processes. Optimization is the process of improving an existing situation, device, or system such as a chemical process. By evaluating a base case, usually a detailed design or an actual process in operation, engineers would have a good starting point and could therefore find strategies to improve the current design/process. The objectives of optimization vary: maximizing revenue, maximizing production rate, minimizing emissions are merely some of these objectives, depend on the type of the plant.

The OM Petrochemical facility has a task of optimizing an ethylbenzene production plant. Given a base case for the production of 99.8 mol% ethylbenzene at 80,000 tonnes per year, our team explored the key components of the facility contributing to the net present value (NPV) of the facility. The main objective of optimization is to maximize the NPV of the plant. According to a previously evaluation of the base case, the team find a NPV of -10 million USD. In order to optimize the process, the team investigated the possible economic advantages of two proposed changes. One proposed change is to use a new catalyst that costs $8/kg compared to the $5/kg catalyst used in the base case simulation. The second proposed change is to use a cheaper feed: a lower grade of benzene feed. During the investigation, these two proposed changes prove themselves to be powerful factors for the entire ethylbenzene production process, and therefore it is vital that we can fully utilize these changes to maximize the plant’s NPV. The team recommended applying both changes in order to optimize the process after scrutinizing the two changes. Other than the two changes, other steps have been taken as well to optimize the process. As a result of optimization, feed flow rate changes and so does the plant's process flow diagram (PFD). The team resized the equipment, and manipulate operating conditions in order to satisfy production requirements and to keep the plant operating in a highly effective and efficient manner. These changes have significant effects on the economics of the plant. The NPV increases to $36 million USD post optimization. In this paper, the author will start from discussing special concerns of operating processes, then present the details of optimization, and elucidate the reasons behind applying these modifications.

Chapter 2
Overview of special concerns

This section focuses on justifying special operating conditions of the ethylbenzene production facility. In order to have an effective process performance, usually temperature, pressure, and other conditions of process streams need to be adjusted. According to Turton, a decision to operate outside the pressure range of 1 to 10 bar, and to operate outside the temperature of 40 to 260 ℃ must be justified. According to the previous study of base case, high temperature and high pressure conditions occur in reactor section, and high temperature differences occur in cooling section. This section will discuss the necessity of operating the process under these conditions, and provide a stepping stone for future optimization measures.

High pressure

When higher pressure conditions present, gas phase reactions tends to have higher reaction rate. Increasing the pressure of a gas, which in turn increases the concentration of the gas, will ultimately increase the reaction rate, because of the fact that the reaction rate is positively correlated to concentration. High pressure could only be beneficial to the plant under certain conditions, however, to prevent higher equipment cost. Reactors need to have thicker walls if the operating pressure is high. Furthermore, gases need to be compressed to high pressure before entering the reactor, therefore high costs due to expensive compressors might be required.

High temperature

The reaction rate is also dependent on temperature. Increasing the temperature will increase reaction rates, because higher temperature increase the number of high energy collisions in atomic level. The reaction kinetics of the involving chemical reactions are of the form:

$$-r_i = f(concentration) * k_o e^{-E/_{RT}}$$

Which can also describe the relationship between temperature and reaction rate.

Temperature condition is facing the same problem with pressure: a high temperature, normally above 400 ℃, requires special materials: the relatively cheaper carbon steel could no longer be applied as they would decompose above 450 ℃ and therefore compromise the effectiveness of the whole plant. Usually, stainless steel is necessary to withstand a high temperature, but equipment made of stainless steel costs much more than carbon steel. There could be an economical penalty for using a temperature higher than 450 ℃.

Non-stoichiometric feed to the reactors

Non-stoichiometric feed is commonly used in industrial reactions because it could help avoid or control side reactions. In order to minimize these additional reactions, the molar ratio of benzene to ethylene fed to the reactors is kept high, at approximately 8:1 in this case. Besides, an excess of one reactant will tend to increase conversion of the other reactant, generally speaking.

Heat exchangers

Heat exchangers operating with large temperature differences is also a concern: even though heat exchangers with large log-mean temperature could better conduct heat integration, this large driving force also means valuable high-temperature energy is wasted. Heat integration is not necessarily profitable.

Chapter 3
Detailed explanation of optimization measures

(1) Reactor section optimization

Length

In the primary investigation of ethylbenzene plant, we observe that raw materials cost plays the most significant role in influencing net present value (NPV). With lower feed flow rate the NPV will decrease dramatically due to the significant amount being consumed every year. In order to decrease the feed flow rate, we take a closer look at the reaction section. In the original plant, the reaction section is composed of a chain of three plug flow reactors, and a fourth reactor is designed for recycle, to maximize the overall conversion of benzene. The team changed the type of catalyst taking advantages of its reaction kinetics, and studied the reactor length and its effects on conversion of benzene as well. Theoretically, longer reactor length means the reactants would have longer time to react with each other, and a higher conversion of reactants would be expected. With side reactions however, longer reactor length could increase the conversion of our desired product to by-product as well, which is not favorable. A case study is therefore necessary and we conducted a simulation using PRO/-II.

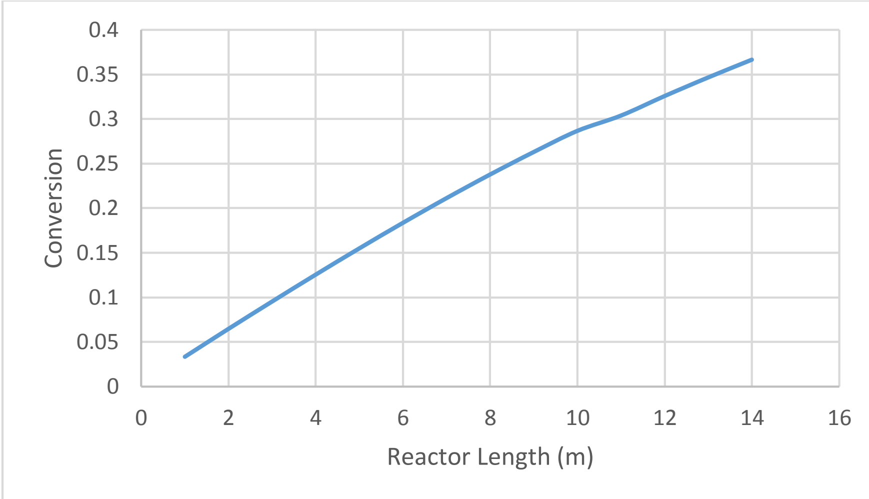

Figure 1: Case Study on reactor length and its effects on conversion of benzene (feed) to ethylbenzene (desired product)

We changed the reactor length while keeping the reactor volume within an acceptable range compared to the reactor sizes in the original design. The reactors must be big enough, so they could achieve an overall high conversion of benzene to ethylbenzene to satisfy the production requirements. The reactors cannot be overwhelmingly large, however, to avoid high expense on purchasing catalyst. Even though a larger reactor would achieve a higher conversion of benzene, we are not expecting any huge equipment which is expensive to build and difficult to take care of. Therefore we decide to use the smallest volumes possible that could produce products that satisfy our needs.

Table 1: Summary of reactor sizes for both base case and optimization

	Length (m)		Volume (m^3)	
	base case	Optimization	base case	Optimization
R301	11	11.0	20	25.6
R302	12	14.5	25	63.5
R303	12	15.7	30	87.1

Pressure and temperature

As mentioned earlier in the report, operating temperature and pressure also have influences on reaction rates and they could affect the feed flow rate as well. In order to prove that high pressure for our reactors would be beneficial, we conduct a case study in PRO/II to study the influences on reactions by changing pressure. We generated two plots: Figure 2, a plot of selectivity of ethylbenzene to diethylbenzene (by-product) vs. Pressure, and Figure 3, a plot of flow rate of diethylbenzene vs. Pressure. From these plots, we could see the trends that higher the pressure, higher the selectivity of the desired product, ethylbenzene, and lower the flow rate of the undesired product, diethylbenzene.

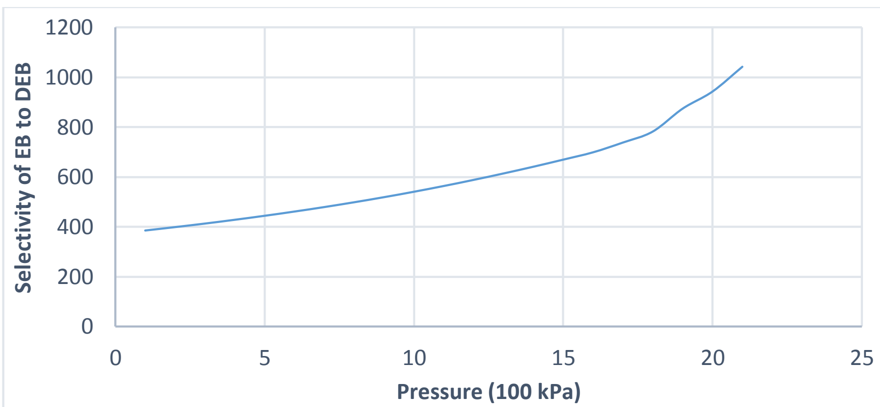

Figure 2: In reactors, pressure affect selectivity of ethylbenzene (desired product) to diethylbenzene (undesired product)

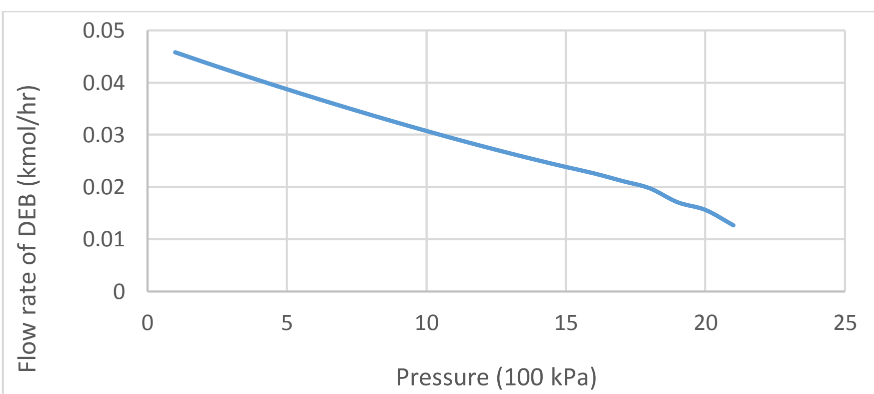

Figure 3: In reactors, pressure have effects on flow rate of undesired product

Considering the possible economic impact of high operating pressure, it is reasonable to choose using a pressure at 2000 kPa for the reactors, in order to achieve relatively higher selectivity of desired product and meanwhile, use less expensive equipment. For our optimization, we decided to use 1900 kPa as the operating pressure.

Higher temperature also increases reaction rates. However, since we are dealing with multiple reactions, we need more complicated calculations.

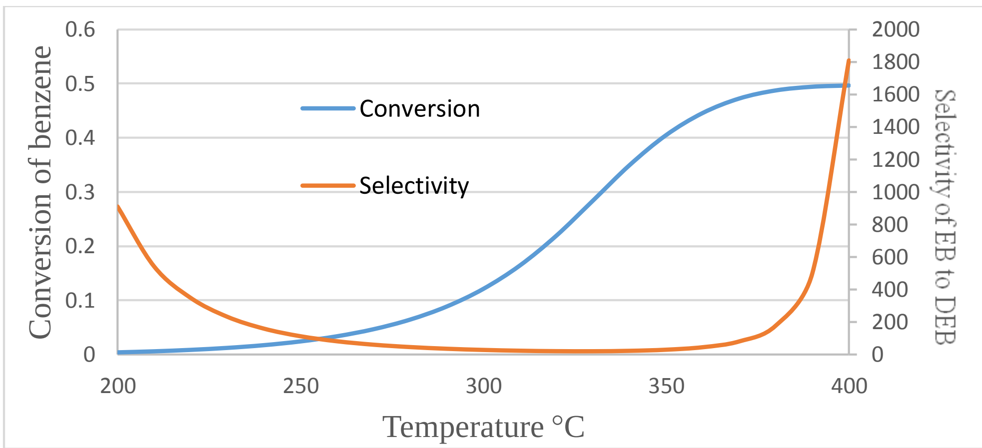

Figure 4: In reactors, temperature have influences on conversion of benzene to ethylbenzene, and also affect selectivity of ethylbenzene to diethylbenzene in product stream

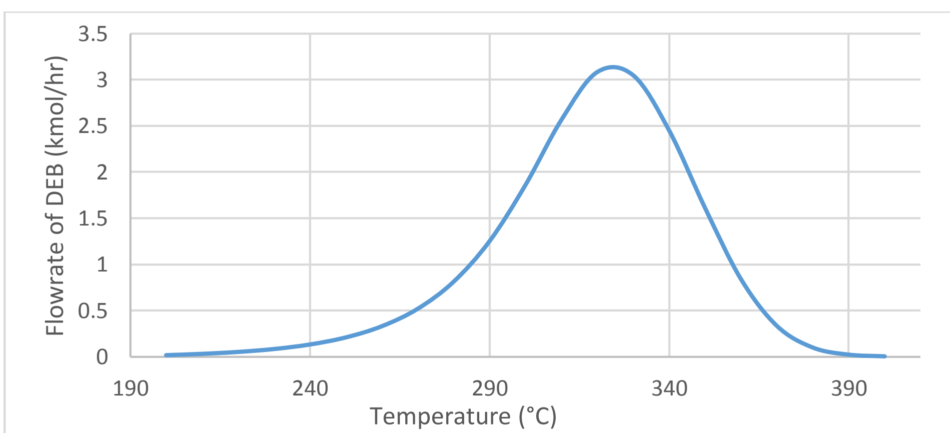

Figure 5: Temperature Effects on Flow Rate of Undesired Product

From the two figures above, we find that both conversion of benzene to ethylbenzene and selectivity of desired product to by-product increase as temperature increases. From Figure 4 we could see that they have higher values when the temperature reaches around 400 ℃. Therefore higher temperature is preferred. It is essential, however, to lower the flow rate of undesired product, to make following separation processes easier to be conducted. From Figure 5, we can see that the flow rate of undesired product reaches its highest point at around 330 ℃. The flow rate becomes lower when temperature keeps on increasing and passes 330 ℃, and the flow rate of the undesired product reaches almost zero as the temperature approaching 390 ℃ or above. We therefore conclude that higher temperature, at least above 390 ℃, is essential for the reactors to operate with higher efficiency: higher conversion, higher selectivity of the desired product, and fewer the undesired product to be produced. If the temperature go beyond around 450 ℃ however, special materials such as stainless steel have to be used as a replacement of carbon steel. Furthermore, reactors are not allowed to operate above 500 ℃ due to the sensitivity of the new catalyst. Therefore throughout our simulation, we increase the reactor inlet temperature, from around 380 ℃ in the base case, to 440 ℃, to increase productivity as much as possible.

Utilizing higher operating temperature and pressure and more efficient catalyst, we are able to produce enough ethylbenzene to eliminate the fourth reactor and associated equipment previously required in the base case simulation; in another word, we manage to simplify the process. The reactor effluent is then sent to a cooling system.

(2) Cooling system optimization

The cooling system contains three heat exchangers in series to condense the vapor effluent from the reactors, preventing flash in the phase separator. While cooling the process stream, these heat exchangers also generate high pressure steam (HPS) or low pressure steam (LPS). HPS and LPS can be sold, thus the plant could obtain credit from selling steam. The plant needs to purchase boiler feed water (BFW) and cooling water (CW): feed BFW to the heat exchangers that could generate steam, and feed CW to the exchanger that is not producing steam. During optimizing heat exchangers, we focused on heat exchanging area and driving force for heat transfer. Since we do not need to be concerned about heat integration, we deliberately increase the driving force by increasing difference in log-mean temperature difference ($\triangle T_{LM}$) inside the heat exchangers. Due to larger $\triangle T_{LM}$, we decrease the areas needed for heat transfer, and therefore the plant can purchase smaller heat exchangers with lower prices. After simulations, we find that the optimization case is making less steam, thus, making less credit comparing to the base case (table 2). Corresponding to larger $\triangle T_{LM}$ however, less amount of boiler feed water and cooling water are being consumed and associated utility cost decreases.

Table 2: A Comparison of cooling system between the base case and optimization. The optimized cooling system of smaller heat exchangers is generating less steam and consuming less cooling water.

	Annual Utility Cost ($/yr)		Area (m^2)	
	Base Case	Optimization	Base Case	Optimization
E-303	-1,807,200	-1,391,300	179	104
E-304	-1,650,000	-1,188,500	502	251
E-305	15,162	6,510	34.3	13.9

(3) Separation unit Optimization:

Pressure of separation vessel

We mount a valve right after the cooling system, to reduce the pressure of the process stream from 1920 kPa to a lower pressure before entering the phase separator that could remove unwanted ethylene, ethane, and propene as fuel gas. We find that we will achieve relatively good separation when pressure in the separation vessel go beyond 600 kPa (figure 6). Therefore, we decided to operate the separator at 600 kPa to minimize the amount of benzene and ethylbenzene in this fuel gas –Ensuring the process does not lose product or benzene that can be recycled back to mix with the feed.

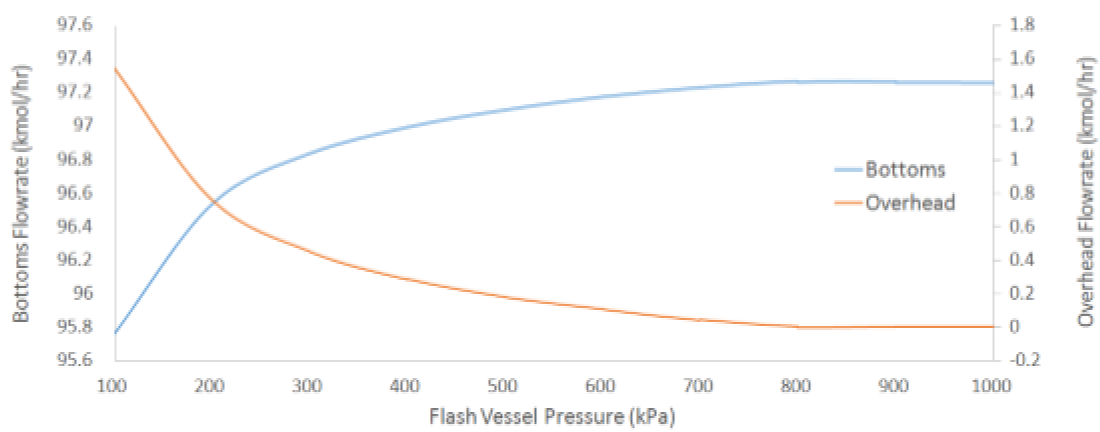

Figure 6: Case Study on separator's operating pressure and its effects on flow rates of effluent streams

Sizing of the vessel

Since the optimized flow rate entering the phase separator is less than that in the base case, we consider to resize the separator to make the plant more economical. The vertical vessel is made of carbon steel, and the optimum ratio of length to diameter is 3. The holdup time for the vessel should be within the range of 5 to 10 minutes. Basing on these heuristics, we design the new vessel with a volume of 3.8 m^3, which is 6.4 m^3 smaller than the vessel in the base case.

Feed for the column

The liquid effluent of the phase separator, containing mostly benzene, ethylbenzene, and some light materials, undergoes a pressure drop via a second valve to 400kPa for entrance into the distillation column. Before deciding to use a second valve, we also considered using a turbine to generate electricity while lowering the pressure of process stream. We decide to use a valve instead of a turbine for two reasons: first, turbines will cause greater heat loss comparing to valves, and the process stream will therefore enter the distillation column at a colder temperature, causing higher energy consumption in the distillation tower; second, turbines are not preferred when process stream contain liquid, and the process stream sending to the column is in fact liquid. We also choose to neglect any further consideration for the turbine after performing an economic analysis. Considering turbines are on average 33% efficient, we validate the use of a valve over a turbine.

Number of trays & feed tray location

The process stream then approaches the distillation column. Sizing the column requires preliminary calculations based on heuristics. The sizing calculations are dependent on stream conditions, physical and chemical properties of the stream, efficiency of trays, energy consumptions of reboiler and condenser, reflux ratio, and many other factors. The simulations eventually give us a column operating with 22 equilibrium trays (27 actual) with a feed tray at no. 19. It is necessary to find an appropriate feed location so that minimum energy consumption would take place in both reboiler and condenser. We choose trays no. 1, 5, 10, 15, and 20 to run simulations and observe duties on condenser and reboiler, and we find at tray no. 5 we achieve a minima: a duty of -12 MM BTU/hr for the condenser. We then choose the feed location at tray no.5 instead of no.19. A partial condenser is used to maintain the vapor state of light materials such as ethane and propene to be separated from the benzene and burned as fuel gas. The overhead liquid draw, benzene, is recycled to mix with the feed, allowing the process to use feed more efficiently. The bottom product stream contains the 99.8 mol% ethylbenzene at the specification of 80,000 tonnes/yr. Since this process meets all the specifications after one column, we are able to remove the second column and associated equipment required in the base case simulation.

Chapter 4
Outcomes

The key advantage to this optimization is utilizing less raw materials while satisfying the requirement of producing 80,000 tonne/yr of the required product. The removal of the second distillation tower and associated equipment also allows for minimization of the duty on the fired heater, reducing the amount of natural gas by nearly half. Equipment removed include a distillation tower, two pumps, and the fourth reactor.

Our proposed optimization also has some disadvantages. The lower concentration of the feed benzene demands the process operate at higher temperatures to force conversion and selectivity to satisfy the requirements. The high temperature and pressure operating conditions used in the reactors require special materials, such as stainless steel, for the process to work in a safe and efficient manner. The cost for purchasing reactors goes significant higher comparing to the base case.

Table 3: Summary of Equipment Cost for both the base case and optimized case

	Base Case	Optimization
Exchangers	$ 1,240,800	$ 920,900
Pumps	$ 216,400	$ 101,500
Heaters	$ 2,460,000	$ 1,960,000
Towers	$ 630,000	$ 739,000
Vessels	$ 209,100	$ 164,500
Reactors	$ 1,174,200	$ 7,350,000
Sum	$ 5,930,500	$ 11,235,900

From sensitivity analysis, equipment pricing does not greatly affect the NPV, cost of raw materials does. In order to compare different costs of the plant throughout the project operating period, we calculate present value of each category. Table 4 and figure 7 shows the present values of different costs for the optimized process. The cost for raw materials takes 74% of the while cost for equipment takes less than 4%.

Table 4: Summary of present values of different costs for the optimized process

Raw materials	$386,761,000
labor	$5,064,000
Catalysts	$2,163,000
Equipment	$18,067,000
Other Costs	$110,343,000
Total	$522,398,000

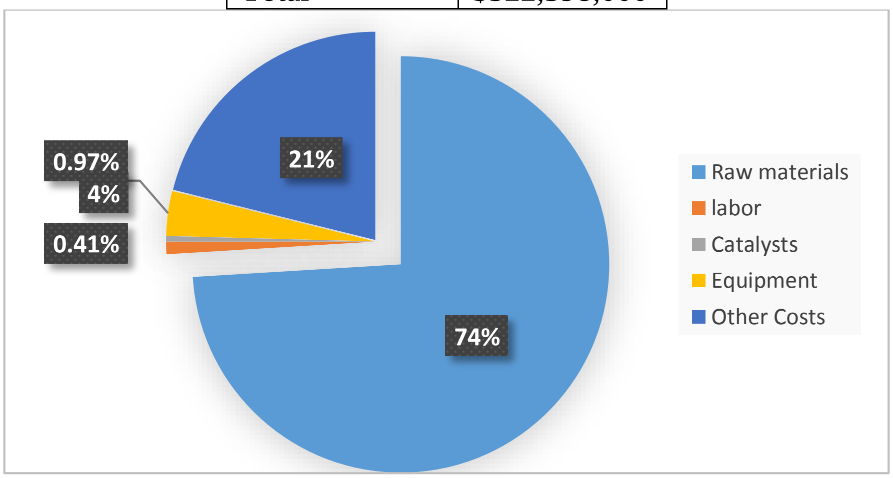

Figure 7: In terms of present value, raw materials cost takes 74% of all the costs for the entire plant

After analyzing economics for the optimization, we conclude that high cost of purchasing equipment is compensated by taking advantages of much lower cost of raw materials. The optimized raw materials cost is $69.9 million/yr, while the cost of raw materials in the base case is $ 85.6 million/yr. We also minimize the use of utilities from $1.9 million/yr to actually making $0.4 million/yr. In the base case simulation of this process, we observed a NPV of -$10 million. This optimization increased NPV dramatically, results in an NPV over the lifespan of the project to be approximately $36.4 million.

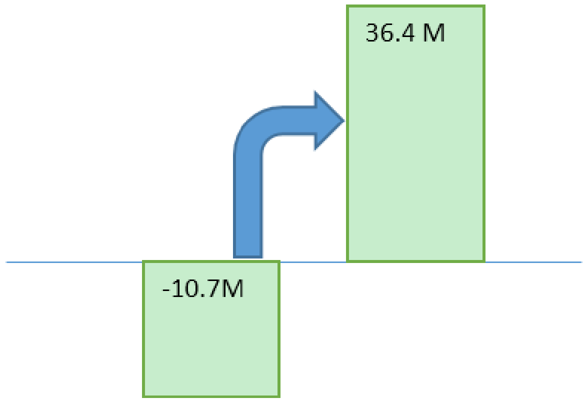

Figure 8: A Comparison of NPV between Base Case and Optimization

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